

# The von Neumann Hierarchy for Correlation Operators of Quantum Many-Particle Systems

*V I Gerasimenko*<sup>†</sup> *V O Shtyk*<sup>‡</sup>

<sup>†</sup> *Institute of Mathematics of NAS of Ukraine*

<sup>‡</sup> *Bogolyubov Institute for Theoretical Physics of NAS of Ukraine*

E-mail: <sup>†</sup> *gerasym@imath.kiev.ua*, <sup>‡</sup> *vshtyk@bitp.kiev.ua*

The Cauchy problem for the von Neumann hierarchy of nonlinear equations is investigated. One describes the evolution of all possible states of quantum many-particle systems by the correlation operators. A solution of such nonlinear equations is constructed in the form of an expansion over particle clusters whose evolution is described by the corresponding order cumulant (semi-invariant) of evolution operators for the von Neumann equations. For the initial data from the space of sequences of trace class operators the existence of a strong and a weak solution of the Cauchy problem is proved. We discuss the relationships of this solution both with the  $s$ -particle statistical operators, which are solutions of the BBGKY hierarchy, and with the  $s$ -particle correlation operators of quantum systems.

*Keywords:* von Neumann hierarchy; BBGKY hierarchy; quantum kinetic equations; cumulant (semi-invariant); cluster expansion; correlation operator; statistical operator (density matrix); quantum many-particle system.

# Contents

<b>1</b>	<b>Introduction</b>	<b>3</b>
<b>2</b>	<b>Evolution equations of quantum many-particle systems</b>	<b>4</b>
2.1	Quantum systems of particles . . . . .	4
2.2	The von Neumann equation . . . . .	5
2.3	Derivation of von Neumann hierarchy for correlation operators . . . . .	6
<b>3</b>	<b>Cluster expansions of evolution operator of von Neumann equation</b>	<b>8</b>
3.1	Cluster expansions . . . . .	8
3.2	Properties of cumulants . . . . .	10
<b>4</b>	<b>Initial-value problem for the von Neumann hierarchy</b>	<b>10</b>
4.1	The formula of a solution . . . . .	10
4.2	Chaos property . . . . .	12
4.3	Properties of a group of nonlinear operators . . . . .	13
4.4	The uniqueness and existence theorem . . . . .	16
<b>5</b>	<b>BBGKY hierarchy</b>	<b>18</b>
5.1	Nonequilibrium grand canonical ensemble . . . . .	18
5.2	On a solution of the BBGKY hierarchy . . . . .	20
5.3	Correlation operators of infinite-particle systems . . . . .	22
	<b>References</b>	<b>24</b>

# 1 Introduction

In the paper we consider the von Neumann hierarchy for correlation operators that describes the evolution of quantum correlations of many-particle systems. The necessity to describe the evolution of correlations arises in many problems of modern statistical mechanics. Among them we refer to such fundamental problems that are challenging for mathematics, in particular, the rigorous derivation of quantum kinetic equations [2, 4–8, 15, 19, 21, 27, 36], for example, the kinetic equations describing Bose gases in the condensate phase [1, 16–18, 35], and the description of nonequilibrium quantum correlations in ultracold Fermi and Bose gases [28](and references therein). In the paper we introduce the hierarchy of equations for correlation operators (the von Neumann hierarchy) that describes the quantum correlations from the microscopic point of view and shows how such dynamics is originated in the dynamics of an infinite-particle system (the BBGKY hierarchy [10, 26, 33]) and nonequilibrium fluctuations of macroscopic characteristics of such systems.

The aim of the work is to formulate the evolution equations describing correlations in quantum many-particle systems with the general type of an interaction potential and construct a solution of the corresponding Cauchy problem, then using the constructed solution to establish its relationships with the solutions of hierarchies of the evolution equations of infinitely many quantum particles.

We outline the structure of the paper and the main results. In section 2 we introduce preliminary facts about the dynamics of quantum systems of non-fixed number of particles and deduce the von Neumann hierarchy for correlation operators which gives the alternative description of the evolution of states of the many-particle systems.

In section 3 we define the cumulants (semi-invariants) of evolution operators of the von Neumann equation and investigate some of their typical properties. It turned out that the concept of cumulants of evolution operators is a basis of the expansions for the solutions of various evolution equations of quantum systems of particles, in particular, the von Neumann hierarchy for correlation operators and the BBGKY hierarchy for infinite-particle systems.

In section 4 the solution of the initial-value problem for the von Neumann hierarchy is constructed and proved that the solution generates a group of nonlinear operators of the class  $C_0$  in the space of trace class operators. In this space we state an existence and uniqueness theorem of a strong and a weak solutions for such a Cauchy problem.

In the last section 5 we discuss the relationships of a solution of the von Neumann hierarchy for correlation operators both with the  $s$ -particle statistical operators, which are solutions of the BBGKY hierarchy and with the  $s$ -particle correlation operators of quantum systems. We also state the general structure of the BBGKY hierarchy generator of infinite-particle quantum systems.

## 2 Evolution equations of quantum many-particle systems

### 2.1 Quantum systems of particles

We consider a quantum system of a non-fixed (i.e. arbitrary but finite) number of identical (spinless) particles with unit mass  $m = 1$  in the space  $\mathbb{R}^\nu$ ,  $\nu \geq 1$  (in the terminology of statistical mechanics it is known as a *nonequilibrium grand canonical ensemble* [11]).

The Hamiltonian of such a system  $H = \bigoplus_{n=0}^{\infty} H_n$  is a self-adjoint operator with domain  $\mathcal{D}(H) = \{\psi = \oplus \psi_n \in \mathcal{F}_{\mathcal{H}} \mid \psi_n \in \mathcal{D}(H_n) \in \mathcal{H}_n, \sum_n \|H_n \psi_n\|^2 < \infty\} \subset \mathcal{F}_{\mathcal{H}}$ ,

where  $\mathcal{F}_{\mathcal{H}} = \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes n}$  is the Fock space over the Hilbert space  $\mathcal{H}$  ( $\mathcal{H}^0 = \mathbb{C}$ ). Assume  $\mathcal{H} = L^2(\mathbb{R}^\nu)$  (coordinate representation) then an element  $\psi \in \mathcal{F}_{\mathcal{H}} = \bigoplus_{n=0}^{\infty} L^2(\mathbb{R}^{\nu n})$

is a sequence of functions  $\psi = (\psi_0, \psi_1(q_1), \dots, \psi_n(q_1, \dots, q_n), \dots)$  such that  $\|\psi\|^2 = |\psi_0|^2 + \sum_{n=1}^{\infty} \int dq_1 \dots dq_n |\psi_n(q_1, \dots, q_n)|^2 < +\infty$ . On the subspace of infinitely differentiable functions with compact supports  $\psi_n \in L_0^2(\mathbb{R}^{\nu n}) \subset L^2(\mathbb{R}^{\nu n})$   $n$ -particle Hamiltonian  $H_n$  acts according to the formula ( $H_0 = 0$ )

$$H_n \psi_n = -\frac{\hbar^2}{2} \sum_{i=1}^n \Delta_{q_i} \psi_n + \sum_{k=1}^n \sum_{i_1 < \dots < i_k=1}^n \Phi^{(k)}(q_{i_1}, \dots, q_{i_k}) \psi_n, \quad (1)$$

where  $\Phi^{(k)}$  is a  $k$ -body interaction potential satisfying Kato conditions [30] and  $\hbar = 2\pi\hbar$  is a Planck constant.

An arbitrary observable of the many-particle system  $A = (A_0, A_1, \dots, A_n, \dots)$  is a sequence of self-adjoint operators  $A_n$  defined on the Fock space  $\mathcal{F}_{\mathcal{H}}$ . We will consider the observables of the system as the elements of the space  $\mathfrak{L}(\mathcal{F}_{\mathcal{H}})$  of sequences of bounded operators with an operator norm [13, 33].

The continuous linear positive functional on the space of observables is defined by the formula

$$\langle A \rangle = (e^a D)_0^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{1, \dots, n} A_n D_n, \quad (2)$$

where  $\text{Tr}_{1, \dots, n}$  is the partial trace over  $1, \dots, n$  particles,  $(e^a D)_0 = \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{1, \dots, n} D_n$  is a normalizing factor (*grand canonical partition function*), for which the notation from section 5 is used. The sequence  $D = (I, D_1, \dots, D_n, \dots)$  is an infinite sequence of self-adjoint positive density operators  $D_n$  ( $I$  is a unit operator) defined on the Fock space  $\mathcal{F}_{\mathcal{H}}$ . This sequence describes the state of a quantum system of non-fixed number of particles. The density operators  $D_n$ ,  $n \geq 1$  (also called *statistical operators* whose kernels are known as *density matrices* [9]), defined on the  $n$ -particle Hilbert space  $\mathcal{H}_n = \mathcal{H}^{\otimes n} = L^2(\mathbb{R}^{\nu n})$ , we will denote by  $D_n(1, \dots, n)$ . For a system of identical particles described by Maxwell-Boltzmann statistics, one has  $D_n(1, \dots, n) = D_n(i_1, \dots, i_n)$  if  $\{i_1, \dots, i_n\} \in \{1, \dots, n\}$ .

We consider the states of a system that belong to the space  $\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}}) = \bigoplus_{n=0}^{\infty} \mathfrak{L}^1(\mathcal{H}_n)$  of sequences  $f = (I, f_1, \dots, f_n, \dots)$  of trace class operators  $f_n = f_n(1, \dots, n) \in \mathfrak{L}^1(\mathcal{H}_n)$ ,

satisfying the above-mentioned symmetry condition, equipped with the trace norm

$$\|f\|_{\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})} = \sum_{n=0}^{\infty} \|f_n\|_{\mathfrak{L}^1(\mathcal{H}_n)} = \sum_{n=0}^{\infty} \text{Tr}_{1,\dots,n} |f_n(1, \dots, n)|.$$

We will denote by  $\mathfrak{L}_0^1$  the everywhere dense set in  $\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  of finite sequences of degenerate operators [30] with infinitely differentiable kernels with compact supports. Note that the space  $\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  contains sequences of operators more general than those determining the states of systems of particles.

For the  $D \in \mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  and  $A \in \mathfrak{L}(\mathcal{F}_{\mathcal{H}})$  functional (2) exists. One is interpreted as an average value (expectation value) of the observable  $A$  in the state with density operator  $D$  (nonequilibrium grand canonical ensemble for the Maxwell-Boltzmann statistics).

We remark that in the case of a system of a fixed number  $N$  of particles (*nonequilibrium canonical ensemble*) the observables and states are the one-component sequences, respectively,  $A^{(N)} = (0, \dots, 0, A_N, 0, \dots)$ ,  $D^{(N)} = (0, \dots, 0, D_N, 0, \dots)$ . Therefore, the formula for an average value reduces to

$$\langle A^{(N)} \rangle = (\text{Tr}_{1,\dots,N} D_N)^{-1} \text{Tr}_{1,\dots,N} A_N D_N.$$

## 2.2 The von Neumann equation

The evolution of all possible states  $D(t) = (I, D_1(t, 1), \dots, D_n(t, 1, \dots, n), \dots)$  is described by the initial-value problem for a sequence of the von Neumann equations (the quantum Liouville equations) [10, 31, 33]

$$\frac{d}{dt} D(t) = -\mathcal{N} D(t), \quad (3)$$

$$D(t)|_{t=0} = D(0), \quad (4)$$

where for  $f \in \mathfrak{L}_0^1(\mathcal{F}_{\mathcal{H}}) \subset \mathcal{D}(\mathcal{N}) \subset \mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  the von Neumann operator is defined by

$$(\mathcal{N}f)_n = -\frac{i}{\hbar} [f_n, H_n] := -\frac{i}{\hbar} (f_n H_n - H_n f_n). \quad (5)$$

In the space of sequences of trace-class operators  $\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  for an abstract initial-value problem (3)–(4) the following theorem is true.

**Theorem 1** ([24, 33]). *The solution of initial-value problem (3)–(4) is determined by the formula*

$$D(t) = \mathcal{U}(-t) D(0) \mathcal{U}^{-1}(-t), \quad (6)$$

where  $\mathcal{U}(-t) = \bigoplus_{n=0}^{\infty} \mathcal{U}_n(-t)$  and

$$\begin{aligned} \mathcal{U}_n(-t) &= e^{-\frac{i}{\hbar} t H_n}, \\ \mathcal{U}_n^{-1}(-t) &= e^{\frac{i}{\hbar} t H_n}, \end{aligned} \quad (7)$$

$\mathcal{U}_0(-t) = I$  is a unit operator.

For  $D(0) \in \mathfrak{L}_0^1(\mathcal{F}_{\mathcal{H}}) \subset \mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  it is a strong (classical) solution and for arbitrary  $D(0) \in \mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  it is a weak (generalized) solution.

Note that the nature of notations (7) used for unitary groups  $e^{\pm \frac{i}{\hbar} t H_n}$  is related to the correspondence principle between quantum and classical systems (for the later the evolution operator for the Liouville equation for the density of the distribution function is defined in analogous terms). It is a consequence of the existence of two approaches to the description of the evolution of systems based on the description of the evolution in framework of observables or states. The evolution operator generated by solution (6) for  $f \in \mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  we will denote by

$$\mathcal{U}(-t)f\mathcal{U}^{-1}(-t) := \mathcal{G}(-t)f. \quad (8)$$

The following properties of the group  $\mathcal{G}(-t)$  follow from the properties of groups (7).

In the space  $\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  the mapping (8) :  $t \rightarrow \mathcal{G}(-t)f$  is an isometric strongly continuous group which preserves positivity and self-adjointness of operators.

For  $f \in \mathfrak{L}_0^1(\mathcal{F}_{\mathcal{H}}) \subset \mathcal{D}(-\mathcal{N})$  in the sense of the norm convergence  $\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  there exists a limit [33] by which the infinitesimal generator:  $-\mathcal{N} = \oplus_{n=0}^{\infty}(-\mathcal{N}_n)$  of the group of evolution operator (8) is determined

$$\lim_{t \rightarrow 0} \frac{1}{t} (\mathcal{G}(-t)f - f) = -\frac{i}{\hbar} (Hf - fH) := -\mathcal{N}f, \quad (9)$$

where  $H = \oplus_{n=0}^{\infty} H_n$  is the Hamiltonian (1) and the operator:  $-\frac{i}{\hbar} (Hf - fH)$  is defined in the domain  $\mathcal{D}(H) \subset \mathcal{F}_{\mathcal{H}}$ .

It should be emphasized that the density operator belonging to the space  $\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  describes only finitely many-particle systems, i.e. systems for which the average number of particles in the system is finite. Indeed, for the observable of the number of particles  $N = (0, I, 2I, \dots, nI, \dots)$  functional (2) has a form

$$\langle N \rangle(t) = (e^a D(0))_0^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{1, \dots, n+1} D_{n+1}(t, 1, \dots, n+1), \quad (10)$$

and for any sequence  $D(t) \in \mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  we get

$$|\langle N \rangle(t)| \leq \|D(0)\|_{\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})} < \infty.$$

## 2.3 Derivation of von Neumann hierarchy for correlation operators

Let us represent the state  $D(t)$  of a quantum system in the form of *cluster expansions* [10, 34] over the new operators  $g(t) = (0, g_1(t, 1), \dots, g_n(t, 1, \dots, n), \dots)$

$$\begin{aligned} D_1(t, 1) &= g_1(t, 1), \\ D_2(t, 1, 2) &= g_2(t, 1, 2) + g_1(t, 1)g_1(t, 2), \\ &\dots\dots\dots \\ D_n(t, Y) &= \sum_{\mathbf{P}: Y = \bigcup_i X_i} \prod_{X_i \subset \mathbb{P}} g_{|X_i|}(t, X_i), \quad n \geq 1, \end{aligned} \quad (11)$$

where the following notations are used:  $Y \equiv (1, \dots, n)$ ,  $|Y| = n$  is a number of particles of the set  $Y$ ,  $\sum_{\mathbf{P}}$  is a sum over all possible partitions  $\mathbf{P}$  of the set  $Y$  into  $|\mathbf{P}|$  nonempty mutually disjoint subsets  $X_i$ .

It is evidently that, in terms of the sequences of operators  $g(t)$ , the state of the system is described in an equivalent way. The operators  $g_n(t)$ ,  $n \geq 1$  are interpreted as *correlation operators* of a system of particles.

The evolution of correlation operators is described by the initial-value problem for the von Neumann hierarchy for correlation operators

$$\frac{d}{dt}g_n(t, Y) = -\mathcal{N}_n(Y)g_n(t, Y) + \sum_{\substack{P: Y=\bigcup X_i, \\ |P|>1}} \left( -\mathcal{N}^{int}(X_1, \dots, X_{|P|}) \right) \prod_{X_i \subset P} g_{|X_i|}(t, X_i), \quad (12)$$

$$g_n(t, Y)|_{t=0} = g_n(0, Y), \quad n \geq 1. \quad (13)$$

The von Neumann operator  $\mathcal{N}_n(Y) = \mathcal{N}_n$  for the system of particles with Hamiltonian (1) is defined by formula (5),

$$\mathcal{N}^{int}(X_1, \dots, X_{|P|}) = \sum_{\substack{Z_1 \subset X_1, \\ Z_1 \neq \emptyset}} \dots \sum_{\substack{Z_{|P|} \subset X_{|P|}, \\ Z_{|P|} \neq \emptyset}} \mathcal{N}_{int}^{(\sum_{r=1}^{|P|} |Z_r|)}(Z_1, \dots, Z_{|P|}), \quad (14)$$

where  $\sum_{Z_j \subset X_j}$  is a sum over all subsets  $Z_j \subset X_j$  and for  $k = 1, \dots, n$

$$\mathcal{N}_{int}^{(k)}(1, 2, \dots, k) = -\frac{i}{\hbar} [\cdot, \Phi^{(k)}(1, 2, \dots, k)]. \quad (15)$$

The simplest examples of von Neumann hierarchy (12) are given by

$$\begin{aligned} \frac{d}{dt}g_1(t, 1) &= -\mathcal{N}_1(1)g_1(t, 1), \\ \frac{d}{dt}g_2(t, 1, 2) &= -\mathcal{N}_2(1, 2)g_2(t, 1, 2) - \mathcal{N}_{int}^{(2)}(1, 2)g_1(t, 1)g_1(t, 2), \\ \frac{d}{dt}g_3(t, 1, 2, 3) &= -\mathcal{N}_3(1, 2, 3)g_3(t, 1, 2, 3) + \\ &+ (-\mathcal{N}_{int}^{(2)}(1, 2) - \mathcal{N}_{int}^{(2)}(1, 3) - \mathcal{N}_{int}^{(3)}(1, 2, 3))g_1(t, 1)g_2(t, 2, 3) + \\ &+ (-\mathcal{N}_{int}^{(2)}(1, 2) - \mathcal{N}_{int}^{(2)}(2, 3) - \mathcal{N}_{int}^{(3)}(1, 2, 3))g_1(t, 2)g_2(t, 1, 3) + \\ &+ (-\mathcal{N}_{int}^{(2)}(1, 3) - \mathcal{N}_{int}^{(2)}(2, 3) - \mathcal{N}_{int}^{(3)}(1, 2, 3))g_1(t, 3)g_2(t, 1, 2) + \\ &- \mathcal{N}_{int}^{(3)}(1, 2, 3)g_1(t, 1)g_1(t, 2)g_1(t, 3). \end{aligned}$$

We note that, in the case of a two-body interaction potential ( $k = 2$ ), the von Neumann hierarchy (12) is simplified. For example, the expression for the operator  $g_3(t)$  does not contain terms with the operator  $\mathcal{N}_{int}^{(3)}$ . In this case the nonlinear terms in hierarchy (12) have the form

$$\sum_{P: Y=X_1 \cup X_2} \sum_{i_1 \in X_1} \sum_{i_2 \in X_2} (-\mathcal{N}_{int}^{(2)}(i_1, i_2))g_{|X_1|}(t, X_1)g_{|X_2|}(t, X_2). \quad (16)$$

For classical systems hierarchy (12) with nonlinear terms (16) is an equivalent form of the corresponding nonlinear Liouville hierarchy [37] formulated by Green [29].

The von Neumann hierarchy (12) can be formally derived from the sequence of (linear) von Neumann equations (3) provided that the state of a system is described in terms of correlation operators defined by cluster expansions (11).

We remark that, in the case of a system of particles satisfying Fermi or Bose statistics, cluster expansions (11) and hierarchy (12) have another structure. The analysis of these cases will be given in a separate paper.

### 3 Cluster expansions of evolution operator of von Neumann equation

#### 3.1 Cluster expansions

Let us expand the group  $\mathcal{G}(-t)$  of evolution operator (8) as follows (*cluster expansions*):

$$\mathcal{G}_n(-t, Y) = \sum_{P: Y = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{|X_i|}(t, X_i), \quad n = |Y| \geq 0, \quad (17)$$

where  $\sum_P$  is the sum over all possible partitions of the set  $Y \equiv (1, \dots, n)$  into  $|P|$  nonempty mutually disjoint subsets  $X_i \subset Y$ . The operators  $\mathfrak{A}_n(t, Y)$  we refer to as the *n*th-order *cumulant (semi-invariant)* of evolution operators (8).

The simplest examples of cluster expansions (17) have the form

$$\begin{aligned} \mathcal{G}_1(-t, 1) &= \mathfrak{A}_1(t, 1), \\ \mathcal{G}_2(-t, 1, 2) &= \mathfrak{A}_2(t, 1, 2) + \mathfrak{A}_1(t, 1) \mathfrak{A}_1(t, 2), \\ \mathcal{G}_3(-t, 1, 2, 3) &= \mathfrak{A}_3(t, 1, 2, 3) + \mathfrak{A}_2(t, 1, 2) \mathfrak{A}_1(t, 3) + \mathfrak{A}_2(t, 1, 3) \mathfrak{A}_1(t, 2) \\ &\quad + \mathfrak{A}_2(t, 2, 3) \mathfrak{A}_1(t, 1) + \mathfrak{A}_1(t, 1) \mathfrak{A}_1(t, 2) \mathfrak{A}_1(t, 3). \end{aligned}$$

Solving previous relations, one obtains

$$\begin{aligned} \mathfrak{A}_1(t, 1) &= \mathcal{G}_1(-t, 1), \\ \mathfrak{A}_2(t, 1, 2) &= \mathcal{G}_2(-t, 1, 2) - \mathcal{G}_1(-t, 1) \mathcal{G}_1(-t, 2), \\ \mathfrak{A}_3(t, 1, 2, 3) &= \mathcal{G}_3(-t, 1, 2, 3) - \mathcal{G}_1(-t, 3) \mathcal{G}_2(-t, 1, 2) - \mathcal{G}_1(-t, 2) \mathcal{G}_2(-t, 1, 3) - \\ &\quad - \mathcal{G}_1(-t, 1) \mathcal{G}_2(-t, 2, 3) + 2! \mathcal{G}_1(-t, 1) \mathcal{G}_1(-t, 2) \mathcal{G}_1(-t, 3). \end{aligned}$$

In general case the following lemma is true.

**Lemma 1.** *A solution of recurrence relations (17) is determined by the expansion*

$$\mathfrak{A}_n(t, Y) = \sum_{P: Y = \bigcup_i X_i} (-1)^{|P|-1} (|P| - 1)! \prod_{X_i \subset P} \mathcal{G}_{|X_i|}(-t, X_i), \quad (18)$$

$$n = |Y| \geq 1,$$

where  $\sum_P$  is the sum over all possible partitions of the set  $Y$  into  $|P|$  nonempty mutually disjoint subsets  $X_i \subset Y$ .



*Proof.* Let us consider the linear space of sequences  $f = (f_0, f_1(1), \dots, f_n(1, \dots, n), \dots)$  of operators  $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$  ( $f_0$  is an operator that multiplies a function by an arbitrary number). We introduce in this linear space the tensor  $*$ -product [20, 34]

$$(f * h)_{|Y|}(Y) = \sum_{Z \subset Y} (f)_{|Z|}(Z) h_{|Y \setminus Z|}(Y \setminus Z), \quad (19)$$

where  $h = (0, h_1(1), \dots, h_n(1, \dots, n), \dots)$  is a sequence of operators  $h_n \in \mathfrak{L}^1(\mathcal{H}_n)$  and  $\sum_{Z \subset Y}$  is the sum over all subsets  $Z$  of the set  $Y \equiv (1, \dots, n)$ .

According to definition (19) for the sequence  $\mathfrak{A}(t) = (0, \mathfrak{A}_1(t, 1), \mathfrak{A}_2(t, 1, 2), \dots, \mathfrak{A}_n(t, 1, \dots, n), \dots)$  the following equality is true

$$\sum_{P: Y = \bigcup_i X_i} \prod_{X_i \subset P} \mathfrak{A}_{(|X_i|)}(t, X_i) = (\mathbb{E} \exp_* \mathfrak{A}(t))_n(Y), \quad n = |Y| \geq 1,$$

where  $\mathbb{E} \exp_*$  is defined as the  $*$ -exponential mapping, i.e.

$$\mathbb{E} \exp_* f = \mathbf{1} + \sum_{n=1}^{\infty} \frac{1}{n!} \underbrace{f * \dots * f}_n, \quad (20)$$

$f \equiv (f_0, f_1, \dots, f_n, \dots)$  and  $\mathbf{1} \equiv (I, 0, 0, \dots)$  is the unit sequence.

As a result, we can represent recurrence relations (17) in the form

$$\mathbf{1} + \tilde{\mathcal{G}}(-t) = \mathbb{E} \exp_* \mathfrak{A}(t),$$

where  $\tilde{\mathcal{G}}(-t) = (0, \mathcal{G}_1(-t, 1), \dots, \mathcal{G}_n(-t, 1, \dots, n), \dots)$  and the elements of the sequence  $\mathcal{G}(-t) \equiv \mathbf{1} + \tilde{\mathcal{G}}(-t) = (I, \mathcal{G}_1(-t, 1), \dots, \mathcal{G}_n(-t, 1, \dots, n), \dots)$  are the evolution operators (8),  $(\mathcal{G}(-t)f)_n(Y) = (\mathcal{U}(-t)f\mathcal{U}^{-1}(-t))_n(Y) = \mathcal{U}_n(-t, Y)f_n(Y)\mathcal{U}_n^{-1}(-t, Y)$  for  $Y = (1, \dots, n)$ .

Similarly, defining the mapping  $\mathbb{L} \exp_*$  on the sequences  $h \equiv (0, h_1, \dots, h_n, \dots)$  as the mapping inverse to  $\mathbb{E} \exp_*$ , i.e.

$$\mathbb{L} \exp_*(\mathbf{1} + h) = \sum_{n=1}^{\infty} \frac{(-1)^{n-1}}{n} \underbrace{h * \dots * h}_n, \quad (21)$$

one obtains

$$\sum_{P: Y = \bigcup_i X_i} (-1)^{|P|-1} (|P| - 1)! \prod_{X_i \subset P} \mathcal{G}_{|X_i|}(-t, X_i) = \mathbb{L} \exp_*(\mathbf{1} + \tilde{\mathcal{G}}(-t))_n(Y),$$

$n = |Y| \geq 1.$

Hence, relation (18) can be rewritten as

$$\mathfrak{A}(t) = \mathbb{L} \exp_*(\mathbf{1} + \tilde{\mathcal{G}}(-t)),$$

and, therefore, expression (18) is a solution of recurrence relations (17).  $\square$

For systems of classical particles cumulants (18) were introduced in [22].

### 3.2 Properties of cumulants

We will now deal with the properties of cumulants (18). As was proved in Lemma 1 the cumulants  $\mathfrak{A}_n(t)$ ,  $n \geq 1$  of evolution operators (8) of the von Neumann equations are solutions of recurrence relations (17), i.e. cluster expansions of the group of evolution operators (8), similar to (11).

For the quantum system of non-interacting particles for  $n \geq 2$  we have:  $\mathfrak{A}_n(t) = 0$ .

Indeed, for a non-interacting Maxwell-Boltzmann gas we have:  $\mathcal{G}_n(-t, 1, \dots, n) = \prod_{i=1}^n \mathcal{G}_1(-t, i)$ , then

$$\begin{aligned} \mathfrak{A}_n(t, Y) &= \sum_{\mathbf{P}: Y = \bigcup_i X_i} (-1)^{|\mathbf{P}|-1} (|\mathbf{P}| - 1)! \prod_{X_i \subset \mathbf{P}} \prod_{j_i=1}^{|X_i|} \mathcal{G}_1(-t, j_i) = \\ &= \sum_{k=1}^n (-1)^{k-1} \mathbf{s}(n, k) (k-1)! \prod_{i=1}^n \mathcal{G}_1(-t, i) = 0. \end{aligned}$$

where the following equality is used:

$$\sum_{\mathbf{P}: Y = \bigcup_i X_i} (-1)^{|\mathbf{P}|-1} (|\mathbf{P}| - 1)! = \sum_{k=1}^n (-1)^{k-1} \mathbf{s}(n, k) (k-1)! = \delta_{n,1}, \quad (22)$$

$\mathbf{s}(n, k)$  is the Stirling numbers of the second kind and  $\delta_{n,1}$  is a Kroneker symbol.

In the general case a generator of the  $n$ th-order cumulant,  $n \geq 2$ , is an operator  $(-\mathcal{N}_{int}^{(n)})$  defined by an  $n$ -body interaction potential (15). According to equality (22) for the  $n$ th-order cumulant,  $n \geq 2$ , in the sense of point-by-point convergence of the space  $\mathfrak{L}^1(\mathcal{H}_n)$  we have

$$\begin{aligned} \lim_{t \rightarrow 0} \frac{1}{t} \mathfrak{A}_n(t, Y) g_n(Y) &= \sum_{\mathbf{P}: Y = \bigcup_k Z_k} (-1)^{|\mathbf{P}|-1} (|\mathbf{P}| - 1)! \sum_{Z_k \subset \mathbf{P}} (-\mathcal{N}_{|Z_k|}(Z_k)) g_n(Y) = \\ &= \left( -\mathcal{N}_{int}^{(n)}(Y) \right) g_n(Y), \quad (23) \end{aligned}$$

where the operator  $\mathcal{N}_{int}^{(n)}$  is given by (15).

For  $n = 1$  the generator of the first-order cumulant is given by

$$\lim_{t \rightarrow 0} \frac{1}{t} (\mathfrak{A}_1(t, Y) - I) g_n(Y) = -\mathcal{N}_n(Y) g_n(Y),$$

where  $Y = (1, \dots, n)$  and  $(-\mathcal{N}_n(Y))$  is defined by formula (9).

## 4 Initial-value problem for the von Neumann hierarchy

### 4.1 The formula of a solution

We consider two approaches to the construction of a solution of the von Neumann hierarchy (12). Since hierarchy (12) has the structure of recurrence equations we deduce

that the solution can be constructed by successive integration of the inhomogeneous von Neumann equations. Indeed, for solutions of the first two equations we have

$$\begin{aligned} g_1(t, 1) &= \mathcal{G}_1(-t, 1)g_1(0, 1), \\ g_2(t, 1, 2) &= \mathcal{G}_2(-t, 1, 2)g_2(0, 1, 2) + \\ &+ \int_0^t dt_1 \mathcal{G}_2(-t + t_1, 1, 2) \left( -\mathcal{N}_{int}^{(2)}(1, 2) \right) \mathcal{G}_1(-t_1, 1) \mathcal{G}_1(-t_1, 2) g_1(0, 1) g_1(0, 2). \end{aligned} \quad (24)$$

Then let us consider the second term on the right hand side of (24)

$$\begin{aligned} &\int_0^t dt_1 \mathcal{G}_2(-t + t_1, 1, 2) \left( -\mathcal{N}_{int}^{(2)}(1, 2) \right) \mathcal{G}_1(-t_1, 1) \mathcal{G}_1(-t_1, 2) = \\ &= -\mathcal{G}_2(-t, 1, 2) \int_0^t dt_1 \frac{d}{dt_1} \left( \mathcal{G}_2(t_1, 1, 2) \mathcal{G}_1(-t_1, 1) \mathcal{G}_1(-t_1, 2) \right) = \\ &= \mathcal{G}_2(-t, 1, 2) - \mathcal{G}_1(-t, 1) \mathcal{G}_1(-t, 2). \end{aligned} \quad (25)$$

The operator  $\mathcal{G}_2(-t, 1, 2) - \mathcal{G}_1(-t, 1) \mathcal{G}_1(-t, 2) := \mathfrak{A}_2(t, 1, 2)$  in (25) is the second-order cumulant of evolution operators (8). Formula (25) is an analog of the Duhamel formula, which holds rigorously, for example, for bounded interaction potential [3].

Making use of the transformations similar to (25), for  $n > 2$  a solution of equations (12), constructed by the iterations is presented by expressions (28).

The formula for a solution of the von Neumann hierarchy (12)–(13) can also be (formally) derived from the solution  $D(t) = (I, D_1(t, 1), \dots, D_n(t, 1, \dots, n), \dots)$  of von Neumann equations (6) (Theorem 1) on the bases of cluster expansions (11).

Indeed, a solution of recurrence equations (11) is defined by the expressions

$$g_n(t, Y) = \sum_{P: Y = \bigcup_i X_i} (-1)^{|P|-1} (|P|-1)! \prod_{X_i \subset P} D_{|X_i|}(t, X_i), \quad n \geq 1, \quad (26)$$

where  $\sum_P$  is a sum over all possible partitions  $P$  of the set  $Y \equiv (1, \dots, n)$  into  $|P|$  nonempty mutually disjoint subsets  $X_i$ . If we substitute solution (6) in expressions (26) and taking into account cluster expansions (11) for  $t = 0$ , we derive

$$g_n(t, Y) = \sum_{P: Y = \bigcup_i X_i} (-1)^{|P|-1} (|P|-1)! \prod_{X_i \subset P} \mathcal{G}_{|X_i|}(-t, X_i) \sum_{P_i: X_i = \bigcup_{k_i} Z_{k_i}} \prod_{Z_{k_i} \subset P_i} g_{|Z_{k_i}|}(0, Z_{k_i}). \quad (27)$$

As a result of the regrouping in expression (27) the items with similar products of initial operators  $\prod_{X_i \subset P} g_{|X_i|}(0, X_i)$ , one obtains

$$g_n(t, Y) = \sum_{P: Y = \bigcup_i X_i} \mathfrak{A}_{|P|}(t, Y_P) \prod_{X_i \subset P} g_{|X_i|}(0, X_i), \quad n \geq 1, \quad (28)$$

where  $Y = (1, \dots, n)$ ,  $Y_P \equiv (X_1, \dots, X_{|P|})$  is a set whose elements are  $|P|$  subsets  $X_i \subset Y$  of partition  $P: Y = \bigcup_i X_i$  and  $\sum_{P: Y = \bigcup_i X_i}$  is a sum over all possible partitions  $P$  of the set  $Y$

into  $|\mathbf{P}|$  nonempty mutually disjoint subsets. Evolution operators  $\mathfrak{A}_{|\mathbf{P}|}(t)$  for every  $|\mathbf{P}| \geq 1$  in expression (28) are defined by

$$\mathfrak{A}_{|\mathbf{P}|}(t, Y_{\mathbf{P}}) := \sum_{\mathbf{P}': Y_{\mathbf{P}} = \bigcup_k Z_k} (-1)^{|\mathbf{P}'|-1} (|\mathbf{P}'| - 1)! \prod_{Z_k \subset \mathbf{P}'} \mathcal{G}_{|Z_k|}(-t, Z_k). \quad (29)$$

For  $|\mathbf{P}| \geq 2$  the  $|\mathbf{P}|$ th-order cumulants  $\mathfrak{A}_{|\mathbf{P}|}(t)$  of evolution operators (8) of the von Neumann equations [25] have similar structure, in contrast to the first-order cumulant. For example, for  $|\mathbf{P}| = 1$

$$\mathfrak{A}_1(t, 1 \cup \dots \cup n) = \mathcal{G}_n(-t, 1, \dots, n),$$

for  $|\mathbf{P}| = 2$

$$\begin{aligned} \mathfrak{A}_2(t, i_1 \cup \dots \cup i_{|X_1|}, i_{|X_1|+1} \cup \dots \cup i_{|Y|}) = \\ = \mathcal{G}_{|Y|}(-t, 1, \dots, n) - \mathcal{G}_{|X_1|}(-t, i_1, \dots, i_{|X_1|}) \mathcal{G}_{|X_2|}(-t, i_{|X_1|+1}, \dots, i_n), \end{aligned}$$

where  $\{i_1, \dots, i_{|Y|}\} \in \{1, \dots, n\}$  and the following notations are used: the symbol  $(i_1 \cup \dots \cup i_{|X_1|}, i_{|X_1|+1} \cup \dots \cup i_{|Y|})$  denote that the sets  $\{i_1, \dots, i_{|X_1|}\}$  and  $\{i_{|X_1|+1}, \dots, i_{|Y|}\}$  are the connected subsets (clusters, respectively, of  $|X_1|$  and  $|X_2|$  particles) of a partition of the set  $Y = (1, \dots, |X_1|, |X_1| + 1, \dots, |Y|)$  into two elements.

The simplest examples for solution (28) are given by

$$\begin{aligned} g_1(t, 1) &= \mathfrak{A}_1(t, 1)g_1(0, 1), \\ g_2(t, 1, 2) &= \mathfrak{A}_1(t, 1 \cup 2)g_2(0, 1, 2) + \mathfrak{A}_2(t, 1, 2)g_1(0, 1)g_1(0, 2), \\ g_3(t, 1, 2, 3) &= \mathfrak{A}_1(t, 1 \cup 2 \cup 3)g_3(0, 1, 2, 3) + \mathfrak{A}_2(t, 2 \cup 3, 1)g_1(0, 1)g_2(0, 2, 3) + \\ &\quad + \mathfrak{A}_2(t, 1 \cup 3, 2)g_1(0, 2)g_2(0, 1, 3) + \mathfrak{A}_2(t, 1 \cup 2, 3)g_1(0, 3)g_2(0, 1, 2) + \\ &\quad + \mathfrak{A}_3(t, 1, 2, 3)g_1(0, 1)g_1(0, 2)g_1(0, 3). \end{aligned}$$

We remark that at the initial instant  $t = 0$  solution (28) satisfies initial condition (13). Indeed, for  $|\mathbf{P}| \geq 2$  according to definitions (7) ( $\mathcal{U}_n^{\pm 1}(0) = I$  is a unit operator) and in view of equality (22), we have

$$\mathfrak{A}_{|\mathbf{P}|}(0, Y_{\mathbf{P}}) = \sum_{\mathbf{P}': Y_{\mathbf{P}} = \bigcup_k Z_k} (-1)^{|\mathbf{P}'|-1} (|\mathbf{P}'| - 1)! I = 0.$$

## 4.2 Chaos property

Let us consider the structure of solution (28) for one physically motivated example of the initial data; that is to say, if the initial data for Cauchy problem (12)–(13) satisfy the chaos property (statistically independent particles) [11], i.e. the sequence of correlation operators is the following one-component sequence

$$g(0) = (0, g_1(0, 1), 0, 0, \dots). \quad (30)$$

In fact, in terms of the sequence  $D(0)$  this condition means that

$$D(0) = (1, D_1(0, 1), D_1(0, 1)D_1(0, 2), \dots).$$

Making use of relation (26) we obtain initial condition (30) for correlation operators. A more general property, namely, decay of correlations for the classical system of hard spheres, was considered in [23].

For initial data (30) the formula for solution (28) of the initial-value problem (12)–(13) is simplified and is reduced to the following formula:

$$g_n(t, 1, \dots, n) = \mathfrak{A}_n(t, 1, \dots, n) \prod_{i=1}^n g_1(0, i), \quad n \geq 1. \quad (31)$$

It is clear from (31) that, if at the initial instant there are no correlations in the system, the correlations generated by the dynamics of a system are completely governed by the cumulants of evolution operators (8).

In the case of initial data (30) solution (31) of the Cauchy problem for the von Neumann hierarchy (12)–(13) may be rewritten in another form. For  $n = 1$ , we have

$$g_1(t, 1) = \mathfrak{A}_1(t, 1)g_1(0, 1).$$

Then, within the context of the definition of the first-order cumulant,  $\mathfrak{A}_1(t)$ , and the inverse to it evolution operator  $\mathfrak{A}_1(-t)$ , we express the correlation operators  $g_n(t)$ ,  $n \geq 2$  in terms of the one-particle correlation operator  $g_1(t)$ , making use of formula (31).

Finally, for  $n \geq 2$  formula (31) is given by

$$g_n(t, 1, \dots, n) = \widehat{\mathfrak{A}}_n(t, 1, \dots, n) \prod_{i=1}^n g_1(t, i), \quad n \geq 2,$$

where  $\widehat{\mathfrak{A}}_n(t, 1, \dots, n)$  is the  $n$ th-order cumulant of the *scattering operators*

$$\widehat{\mathcal{G}}_t(1, \dots, n) := \mathcal{G}_n(-t, 1, \dots, n) \prod_{k=1}^n \mathcal{G}_1(t, k), \quad n \geq 1.$$

The generator of the scattering operator  $\widehat{\mathcal{G}}_t(1, \dots, n)$  is determined by the operator:

$$-\sum_{k=2}^n \sum_{i_1 < \dots < i_k=1}^n \mathcal{N}_{int}^{(k)}(i_1, \dots, i_k),$$

where  $\mathcal{N}_{int}^{(k)}$  acts according to (15).

### 4.3 Properties of a group of nonlinear operators

On  $\mathfrak{L}^1(\mathcal{H}_n)$  solution (28) generates a group of nonlinear operators of the von Neumann hierarchy. The properties of this group are described in the following theorem.

**Theorem 2.** For  $g_n \in \mathfrak{L}^1(\mathcal{H}_n)$ ,  $n \geq 1$ , the mapping

$$t \rightarrow \left( \mathfrak{A}_t(g) \right)_n(Y) \equiv \sum_{\mathbf{P}: Y = \bigcup_i X_i} \mathfrak{A}_{|\mathbf{P}|}(t, Y_{\mathbf{P}}) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) \quad (32)$$

is a group of nonlinear operators of class  $C_0$ . In the subspace  $\mathfrak{L}_0^1(\mathcal{H}_n) \subset \mathfrak{L}^1(\mathcal{H}_n)$  the infinitesimal generator  $\mathcal{N}^{nl}(\cdot)$  of group (32) is defined by the operator

$$(\mathcal{N}^{nl}(g))_n(Y) := -\mathcal{N}_n(Y)g_n(Y) + \sum_{\substack{\mathbf{P}: Y=\bigcup_i X_i, \\ |\mathbf{P}|>1}} \left( -\mathcal{N}^{int}(X_1, \dots, X_{|\mathbf{P}|}) \right) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i), \quad (33)$$

where the notations are similar to those in (14).

*Proof.* Mapping (32) is defined for  $g_n \in \mathfrak{L}^1(\mathcal{H}_n)$ ,  $n \geq 1$  and the following inequality holds:

$$\|(\mathfrak{A}_t(g))_n\|_{\mathfrak{L}^1(\mathcal{H}_n)} \leq n!e^{2n+1}c^n, \quad (34)$$

where  $c := \max_{\mathbf{P}: Y=\bigcup_i X_i} \|g_{|X_i|}(X_i)\|_{\mathfrak{L}^1(\mathcal{H}_{|X_i|})}$ .

Indeed, inasmuch as for  $g_n \in \mathfrak{L}^1(\mathcal{H}_n)$  the equality holds [24]

$$\text{Tr}_{1,\dots,n} |\mathcal{G}_n(-t)g_n| = \|g_n\|_{\mathfrak{L}^1(\mathcal{H}_n)},$$

we have

$$\begin{aligned} \|(\mathfrak{A}_t(g))_n\|_{\mathfrak{L}^1(\mathcal{H}_n)} &\leq \sum_{\mathbf{P}: Y=\bigcup_i X_i} \sum_{\mathbf{P}': Y_{\mathbf{P}}=\bigcup_k Z_k} (|\mathbf{P}'| - 1)! \prod_{X_i \subset \mathbf{P}} \|g_{|X_i|}\|_{\mathfrak{L}^1(\mathcal{H}_{|X_i|})} \leq \\ &\leq \sum_{\mathbf{P}: Y=\bigcup_i X_i} c^{|\mathbf{P}|} \sum_{k=1}^{|\mathbf{P}|} s(|\mathbf{P}|, k)(k-1)! \leq \sum_{\mathbf{P}: Y=\bigcup_i X_i} c^{|\mathbf{P}|} \sum_{k=1}^{|\mathbf{P}|} k^{|\mathbf{P}|-1} \leq n!e^{2n+1}c^n, \end{aligned}$$

where  $s(|\mathbf{P}|, k)$  are the Stirling numbers of the second kind. That is,  $(\mathfrak{A}_t(g))_n \in \mathfrak{L}^1(\mathcal{H}_n)$  for arbitrary  $t \in \mathbb{R}^1$  and  $n \geq 1$ .

We can now formulate the group property of the one-parametric family of nonlinear operators  $\mathfrak{A}_t(\cdot)$  which are defined by (32), i.e.

$$\mathfrak{A}_{t_1}(\mathfrak{A}_{t_2}(g)) = \mathfrak{A}_{t_2}(\mathfrak{A}_{t_1}(g)) = \mathfrak{A}_{t_1+t_2}(g).$$

Indeed, for  $g_n \in \mathfrak{L}^1(\mathcal{H}_n)$ ,  $n \geq 1$  and for any  $t_1, t_2 \in \mathbb{R}^1$ , according to (28) and (18), we have

$$\begin{aligned} (\mathfrak{A}_{t_1}(\mathfrak{A}_{t_2}(g)))_n(Y) &= \sum_{\mathbf{P}: Y=\bigcup_i X_i} \mathfrak{A}_{|\mathbf{P}|}(t_1, Y_{\mathbf{P}}) \prod_{X_i \subset \mathbf{P}} \sum_{\mathbf{P}_i: X_i=\bigcup_{l_i} Z_{l_i}} \mathfrak{A}_{|\mathbf{P}_i|}(t_2, \{X_i\}_{\mathbf{P}_i}) \prod_{Z_{l_i} \subset \mathbf{P}_i} g_{|Z_{l_i}|}(Z_{l_i}) = \\ &= \sum_{\mathbf{P}: Y=\bigcup_i X_i} \sum_{\mathbf{P}': Y_{\mathbf{P}}=\bigcup_j Q_j} (-1)^{|\mathbf{P}'|-1} (|\mathbf{P}'| - 1)! \prod_{Q_j \subset \mathbf{P}'} \mathcal{G}_{|Q_j|}(-t_1, Q_j) \times \\ &\times \prod_{X_i \subset \mathbf{P}} \sum_{\mathbf{P}_i: X_i=\bigcup_{l_i} Z_{l_i}} \sum_{\mathbf{P}'_i: \{X_i\}_{\mathbf{P}_i}=\bigcup_{k_i} R_{k_i}} (-1)^{|\mathbf{P}'_i|-1} (|\mathbf{P}'_i| - 1)! \prod_{R_{k_i} \subset \mathbf{P}'_i} \mathcal{G}_{|R_{k_i}|}(-t_2, R_{k_i}) \prod_{Z_{l_i} \subset \mathbf{P}_i} g_{|Z_{l_i}|}(Z_{l_i}), \end{aligned}$$

where  $\{X_i\}_{\mathbf{P}_i} \equiv (Z_1, \dots, Z_{|\mathbf{P}_i|})$  is a set whose elements are  $|\mathbf{P}_i|$  subsets  $Z_{l_i} \subset X_i$  of the partition  $\mathbf{P}_i: X_i = \bigcup_{l_i} Z_{l_i}$ . Having collected the items at identical products of the initial

data  $g_n(0)$ ,  $n \geq 1$ , and taking into account the group property of the evolution operators  $\mathcal{U}_n^{\pm 1}(-t)$ ,  $n \geq 1$  (7), we obtain

$$\begin{aligned} (\mathfrak{A}_{t_1}(\mathfrak{A}_{t_2}(g)))_n(Y) &= \sum_{\mathbf{P}: Y=\bigcup_i X_i} \sum_{\mathbf{P}': Y_{\mathbf{P}}=\bigcup_k Q_k} (-1)^{|\mathbf{P}'|-1} (|\mathbf{P}'|-1)! \prod_{Q_k \subset \mathbf{P}'} \mathcal{G}_{|Q_k|}(-t_1-t_2, Q_k) \times \\ &\times \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) = \sum_{\mathbf{P}: Y=\bigcup_i X_i} \mathfrak{A}_{|\mathbf{P}|}(t_1+t_2, Y_{\mathbf{P}}) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) = (\mathfrak{A}_{t_1+t_2}(g))_n(Y). \end{aligned}$$

Similarly, we establish

$$\mathfrak{A}_{t_2}(\mathfrak{A}_{t_1}(g)) = \mathfrak{A}_{t_1+t_2}(g).$$

The strong continuity property of the group  $\mathfrak{A}_t(g(0))$  over the parameter  $t \in \mathbb{R}^1$  is a consequence of the strong continuity of group (8) of the von Neumann equations [13]. Indeed, according to identity (22) the following equality holds

$$\sum_{\mathbf{P}: Y=\bigcup_i X_i} \sum_{\mathbf{P}': Y_{\mathbf{P}}=\bigcup_k Z_k} (-1)^{|\mathbf{P}'|-1} (|\mathbf{P}'|-1)! \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) = g_n(Y).$$

Therefore, for  $g_n \in \mathfrak{L}_0^1(\mathcal{H}_n) \subset \mathfrak{L}^1(\mathcal{H}_n)$ ,  $n \geq 1$ , we have

$$\begin{aligned} &\lim_{t \rightarrow 0} \left\| \sum_{\mathbf{P}: Y=\bigcup_i X_i} \sum_{\mathbf{P}': Y_{\mathbf{P}}=\bigcup_k Z_k} (-1)^{|\mathbf{P}'|-1} (|\mathbf{P}'|-1)! \prod_{Z_k \subset \mathbf{P}'} \mathcal{G}_{|Z_k|}(-t, Z_k) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) - g_n(Y) \right\|_{\mathfrak{L}^1(\mathcal{H}_n)} \\ &\leq \sum_{\mathbf{P}: Y=\bigcup_i X_i} \sum_{\mathbf{P}': Y_{\mathbf{P}}=\bigcup_k Z_k} (|\mathbf{P}'|-1)! \lim_{t \rightarrow 0} \left\| \prod_{Z_k \subset \mathbf{P}'} \mathcal{G}_{|Z_k|}(-t, Z_k) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) - \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) \right\|_{\mathfrak{L}^1(\mathcal{H}_n)}. \end{aligned}$$

In view of the fact that group  $\mathcal{G}_n(-t)$  (8) (Theorem 1) is a strong continuous, i.e. in the sense of the norm convergence  $\mathfrak{L}^1(\mathcal{H}_n)$  there exists the limit

$$\lim_{t \rightarrow 0} (\mathcal{G}_n(-t)g_n - g_n) = 0,$$

which implies that, for mutually disjoint subsets  $X_i \subset Y$ , the following equality is also valid:

$$\lim_{t \rightarrow 0} \left( \prod_{Z_k \subset \mathbf{P}'} \mathcal{G}_{|Z_k|}(-t, Z_k) g_n - g_n \right) = 0.$$

For  $g_n \in \mathfrak{L}_0^1(\mathcal{H}_n) \subset \mathfrak{L}^1(\mathcal{H}_n)$ , we finally have

$$\lim_{t \rightarrow 0} \|(\mathfrak{A}_t(g))_n - g_n\|_{\mathfrak{L}^1(\mathcal{H}_n)} = 0.$$

We will now construct the generator  $\mathcal{N}^{nl}(\cdot)$  of group (32). Taking into account that for  $g_n \in \mathfrak{L}_0^1(\mathcal{H}_n) \subset \mathcal{D}(\mathcal{N}_n^{nl}(\cdot))$  equality (9) holds, let us differentiate the group  $(\mathfrak{A}_t(g))_n \psi_n$  for

all  $\psi_n \in \mathcal{D}(H_n) \subset \mathcal{H}_n$ . According to equality (23) for the  $|\mathbf{P}|$ th-order cumulant,  $|\mathbf{P}| \geq 2$ , we obtain

$$\begin{aligned} \lim_{t \rightarrow 0} \frac{1}{t} \mathfrak{A}_{|\mathbf{P}|}(t, Y_{\mathbf{P}}) g_n \psi_n &= \sum_{\mathbf{P}': Y_{\mathbf{P}} = \bigcup_k Z_k} (-1)^{|\mathbf{P}'|-1} (|\mathbf{P}'| - 1)! \sum_{Z_k \subset \mathbf{P}'} (-\mathcal{N}_{|Z_k|}(Z_k)) g_n \psi_n = \\ &= \sum_{\substack{Z_1 \subset X_1, \\ Z_1 \neq \emptyset}} \dots \sum_{\substack{Z_{|\mathbf{P}|} \subset X_{|\mathbf{P}|}, \\ Z_{|\mathbf{P}|} \neq \emptyset}} \left( -\mathcal{N}_{int}^{\left(\sum_{r=1}^{|\mathbf{P}|} |Z_r|\right)}(Z_1, \dots, Z_{|\mathbf{P}|}) \right) g_n \psi_n = \left( -\mathcal{N}^{int}(Y_{\mathbf{P}}) \right) g_n \psi_n, \end{aligned}$$

where  $Y_{\mathbf{P}} \equiv (X_1, \dots, X_{|\mathbf{P}|})$  is a set whose elements are  $|\mathbf{P}|$  subsets  $X_i \subset Y$  of partition  $\mathbf{P} : Y = \bigcup_i X_i$  and the operator  $\mathcal{N}_{int}^{(n)}$  is given by formula (15).

Therefore, for group (32) we derive

$$\begin{aligned} \lim_{t \rightarrow 0} \frac{1}{t} \left( (\mathfrak{A}_t(g))_n - g_n \right) \psi_n &= \lim_{t \rightarrow 0} \frac{1}{t} \left( \sum_{\mathbf{P}: Y = \bigcup_i X_i} \mathfrak{A}_{|\mathbf{P}|}(t, Y_{\mathbf{P}}) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) - g_n(Y) \right) \psi_n = \\ &= \lim_{t \rightarrow 0} \frac{1}{t} (\mathfrak{A}_1(t, Y) g_n - g_n) \psi_n + \sum_{\substack{\mathbf{P}: Y = \bigcup_i X_i, \\ |\mathbf{P}| > 1}} \lim_{t \rightarrow 0} \frac{1}{t} \mathfrak{A}_{|\mathbf{P}|}(t, Y_{\mathbf{P}}) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) \psi_n = \\ &= (-\mathcal{N}_n g_n)(Y) \psi_n + \sum_{\substack{\mathbf{P}: Y = \bigcup_i X_i, \\ |\mathbf{P}| > 1}} \left( -\mathcal{N}^{int}(Y_{\mathbf{P}}) \right) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(X_i) \psi_n. \quad (35) \end{aligned}$$

Then in view of equality (35) and the proof of the theorem 2 for  $g_n \in \mathfrak{L}_0^1(\mathcal{H}_n) \subset \mathcal{D}(\mathcal{N}_n^{nl}(\cdot)) \subset \mathfrak{L}^1(\mathcal{H}_n)$ ,  $n \geq 1$ , in the sense of the norm convergence in  $\mathfrak{L}^1(\mathcal{H}_n)$ , we finally have

$$\lim_{t \rightarrow 0} \left\| \frac{1}{t} \left( (\mathfrak{A}_t(g))_n - g_n \right) - (\mathcal{N}^{nl}(g))_n \right\|_{\mathfrak{L}^1(\mathcal{H}_n)} = 0,$$

where  $\mathcal{N}^{nl}(\cdot)$  is given by formula (33). □

#### 4.4 The uniqueness and existence theorem

For abstract initial-value problem (12)–(13) in the space  $\mathfrak{L}^1(\mathcal{H}_n)$  of trace class operators the following theorem holds.

**Theorem 3.** *The solution of initial-value problem (12)–(13) for the von Neumann hierarchy (12) is determined by formula (28). For  $g_n(0) \in \mathfrak{L}_0^1(\mathcal{H}_n) \subset \mathfrak{L}^1(\mathcal{H}_n)$  it is a strong (classical) solution and for arbitrary initial data  $g_n(0) \in \mathfrak{L}^1(\mathcal{H}_n)$  it is a weak (generalized) solution.*

*Proof.* According to theorem 2 for initial data  $g_n(0) \in \mathfrak{L}_0^1(\mathcal{H}_n) \subset \mathfrak{L}^1(\mathcal{H}_n)$ ,  $n \geq 1$ , sequence (28) is a strong solution of initial-value problem (12)–(13).



Let us show that in the general case  $g(0) \in \mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  expansions (28) give a weak solution of the initial-value problem for the von Neumann hierarchy (12). Consider the functional

$$(\varphi_n, g_n(t)) := \text{Tr}_{1,\dots,n} \varphi_n g_n(t), \quad (36)$$

where  $\varphi_n \in \mathfrak{L}_0(\mathcal{H}_n)$  are degenerate bounded operators with infinitely times differentiable kernels with compact supports. The operator  $g_n(t)$  is defined by (28) for the arbitrary initial data  $g_k(0) \in \mathfrak{L}^1(\mathcal{H}_k)$ ,  $k = 1, \dots, n$ . According to estimate (34) for  $g_n \in \mathfrak{L}^1(\mathcal{H}_n)$  and  $\varphi_n \in \mathfrak{L}_0(\mathcal{H}_n)$  functional (36) exists.

We transform functional (36) as follows

$$\begin{aligned} (\varphi_n, g_n(t)) &= \sum_{\mathbf{P}: Y = \bigcup_i X_i} \left( \varphi_n, \mathfrak{A}_{|\mathbf{P}|}(t, Y_{\mathbf{P}}) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(0, X_i) \right) = \\ &= \sum_{\mathbf{P}: Y = \bigcup_i X_i} \sum_{\mathbf{P}': Y_{\mathbf{P}'} = \bigcup_k Z_k} (-1)^{|\mathbf{P}'|-1} (|\mathbf{P}'| - 1)! \left( \prod_{Z_k \subset \mathbf{P}'} \mathcal{G}_{|Z_k|}(t; Z_k) \varphi_n, \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(0, X_i) \right), \end{aligned} \quad (37)$$

where the group of operators  $\mathcal{G}_n(t)$  is adjoint to the group  $\mathcal{G}_n(-t)$  in the sense of functional (36).

For  $g_n(0) \in \mathfrak{L}^1(\mathcal{H}_n)$  and  $\varphi_n \in \mathfrak{L}_0(\mathcal{H}_n)$  within the context of the theorem 2 we have

$$\lim_{t \rightarrow 0} \left( \left( \frac{1}{t} (\mathcal{G}_n(t) \varphi_n - \varphi_n), g_n(0) \right) - (\mathcal{N}_n \varphi_n, g_n(0)) \right) = 0,$$

and, therefore, it holds that

$$\begin{aligned} \lim_{t \rightarrow 0} \left( \frac{1}{t} \left( \prod_{Z_k \subset \mathbf{P}'} \mathcal{G}_{|Z_k|}(t; Z_k) \varphi_n - \varphi_n \right), \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(0, X_i) \right) &= \\ &= \left( \sum_{Z_l \subset \mathbf{P}'} \mathcal{N}_{|Z_l|}(Z_l) \varphi_n, \prod_{Z_k \subset \mathbf{P}'} \mathcal{G}_{|Z_k|}(-t; Z_k) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(0, X_i) \right). \end{aligned}$$

Then, for representation (37) of functional (36), one obtains

$$\begin{aligned} \frac{d}{dt} (\varphi_n, g_n(t)) &= (\mathcal{N}_n \varphi_n, g_n(t)) + \sum_{\substack{\mathbf{P}: Y = \bigcup_i X_i, \\ |\mathbf{P}| > 1}} \sum_{\mathbf{P}': Y_{\mathbf{P}'} = \bigcup_k Z_k} (-1)^{|\mathbf{P}'|-1} (|\mathbf{P}'| - 1)! \times \\ &\times \left( \sum_{Z_l \subset \mathbf{P}'} \mathcal{N}_{|Z_l|}(Z_l) \varphi_n, \prod_{Z_k \subset \mathbf{P}'} \mathcal{G}_{|Z_k|}(-t; Z_k) \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(0, X_i) \right) = \\ &= (\mathcal{N}_n \varphi_n, g_n(t)) + \sum_{\substack{\mathbf{P}: Y = \bigcup_i X_i, \\ |\mathbf{P}| > 1}} \left( \mathcal{N}^{int}(X_1, \dots, X_{|\mathbf{P}|}) \varphi_n, \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(t, X_i) \right), \end{aligned}$$

where the operator  $\mathcal{N}^{int}(X_1, \dots, X_{|\mathbf{P}|})$  is defined by (14) and (15).

For functional (36) we finally have

$$\begin{aligned} \frac{d}{dt} (\varphi_n, g_n(t)) &= \\ &= \left( (\mathcal{N}_n \varphi_n)(Y), g_n(t, Y) \right) + \sum_{\substack{\mathbf{P}: Y = \bigcup_i X_i, \\ |\mathbf{P}| > 1}} \left( \mathcal{N}^{int}(X_1, \dots, X_{|\mathbf{P}|}) \varphi_n, \prod_{X_i \subset \mathbf{P}} g_{|X_i|}(t, X_i) \right). \end{aligned} \quad (38)$$

Equality (38) means that for arbitrary initial data  $g_n(0) \in \mathcal{L}^1(\mathcal{H}_n)$ ,  $n \geq 1$ , the weak solution of the initial-value problem of the von Neumann hierarchy (12)–(13) is determined by formula (28).  $\square$

## 5 BBGKY hierarchy

### 5.1 Nonequilibrium grand canonical ensemble

As we have seen above the two equivalent approaches to the description of the state evolution of quantum many-particle systems were formulated, namely, both on the basis of von Neumann equations (3) for the statistical operators  $D(t)$  and of the von Neumann hierarchy (12) for the correlation operators  $g(t)$ . For the system of a finite average number of particles there exists another possibility to describe the evolution of states, namely, by sequences of  $s$ -particle statistical operators that satisfy the BBGKY hierarchy [10].

Traditionally such a hierarchy is deduced on the basis of solutions of the von Neumann equations (the nonequilibrium grand canonical ensemble [11, 25, 33] or the canonical ensemble [2, 10, 15]) in the space of sequences of trace class operators.

The sequence  $F(t) = (I, F_1(t, 1), \dots, F_s(t, 1, \dots, s), \dots)$  of  $s$ -particle statistical operators  $F_s(t, 1, \dots, s)$ ,  $s \geq 1$  can be defined in the framework of the sequence of operators  $D(t) = (I, D_1(t, 1), \dots, D_n(t, 1, \dots, n), \dots)$  (the operator  $D_n(t)$  being regarded as density operator (6) of the  $n$ -particle system) by expressions [33]

$$F_s(t, 1, \dots, s) = (e^a D(0))_0^{-1} \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{s+1, \dots, s+n} D_{s+n}(t, 1, \dots, s+n), \quad s \geq 1, \quad (39)$$

where  $(e^a D(0))_0 = 1 + \sum_{n=1}^{\infty} \frac{1}{n!} \text{Tr}_{1, \dots, n} D_n(0, 1, \dots, n)$  is a partition function (see definition of functional (2)). For  $D(0) \in \mathcal{L}^1(\mathcal{F}_{\mathcal{H}})$  series (39) converges.

If we describe the states of a quantum system of particles in the framework of correlation operators  $g(t)$  the  $s$ -particle statistical operators, that are solutions of the BBGKY hierarchy, are defined by the expansion

$$F_s(t, 1, \dots, s) = \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{s+1, \dots, s+n} g_{1+n}(t, 1 \cup \dots \cup s, s+1, \dots, s+n), \quad s \geq 1, \quad (40)$$

where  $g_{1+n}(t, 1 \cup \dots \cup s, s+1, \dots, s+n)$ ,  $n \geq 0$ , are correlation operators (28) that satisfy the von Neumann hierarchy (12) for a system consisting both from particles and the cluster of  $s$  particles ( $1 \cup \dots \cup s$  is a notation as to formula (29)).

Expansion (40) can be derived from (39) as a result of the following representation for right hand side of expansion (39)

$$\begin{aligned} F_s(t, 1, \dots, s) &= \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{s+1, \dots, s+n} \sum_{\mathbf{P}: \{1 \cup \dots \cup s, s+1, \dots, s+n\} = \bigcup_i X_i} (-1)^{|\mathbf{P}|-1} (|\mathbf{P}|-1)! \prod_{X_i \subset \mathbf{P}} D_{|X_i|}(t, X_i), \quad s \geq 1, \end{aligned} \quad (41)$$

where  $\sum_P$  is a sum over all possible partitions  $P$  of the set  $\{1 \cup \dots \cup s, s+1, \dots, s+n\}$  into  $|P|$  nonempty mutually disjoint subsets  $X_i$ . If  $D(t) \in \mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$  series (41) converges.

We remark that expansion (39) can be defined for more general class of operators then from the space  $\mathfrak{L}^1(\mathcal{F}_{\mathcal{H}})$ .

To prove representation (41) we will first introduce some necessary facts. We will use the notations of lemma 1. According to the definition of  $*$ -product (19) for the sequence  $f = (f_0, f_1(1), f_2(1, 2), \dots, f_n(1, \dots, n), \dots)$  of elements  $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$  the mapping  $\mathbb{E}xp_*$  is defined by series (20). The mapping  $\mathbb{L}n_*$  that inverse to  $\mathbb{E}xp_*$  is defined by series (21).

For  $f = (f_0, f_1, \dots, f_n, \dots)$ ,  $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$  we define the mapping  $\mathfrak{d}_1 : f \rightarrow \mathfrak{d}_1 f$  by

$$(\mathfrak{d}_1 f)_n(1, \dots, n) := f_{n+1}(1, \dots, n, n+1), \quad n \geq 0,$$

and for arbitrary set  $Y = (1, \dots, s)$  we define the linear mapping  $\mathfrak{d}_1 \dots \mathfrak{d}_s : f \rightarrow \mathfrak{d}_1 \dots \mathfrak{d}_s f$  by

$$(\mathfrak{d}_1 \dots \mathfrak{d}_s f)_n := f_{s+n}(1, \dots, s+n). \quad (42)$$

We note that for sequences  $f^1 = (f_0^1, f_1^1, \dots, f_n^1, \dots)$ ,  $f_n^1 \in \mathfrak{L}^1(\mathcal{H}_n)$  and  $f^2 = (f_0^2, f_1^2, \dots, f_n^2, \dots)$ ,  $f_n^2 \in \mathfrak{L}^1(\mathcal{H}_n)$  the following identity holds [34]

$$\mathfrak{d}_1(f^1 * f^2) = \mathfrak{d}_1 f^1 * f^2 + f^1 * \mathfrak{d}_1 f^2.$$

Further, since  $Y_P = (X_1, \dots, X_{|P|})$  then  $Y_1 = (1 \cup \dots \cup s)$  (cluster of  $s$  particles) is one element ( $|Y_1| = 1$ ) of the partition  $P$  ( $|P| = 1$ ), we introduce the mapping  $\mathfrak{d}_{Y_1} : f \rightarrow \mathfrak{d}_{Y_1} f$ , as follows

$$(\mathfrak{d}_{Y_1} f)_n(1, \dots, n) = f_{n+1}(Y_1, 1, \dots, n), \quad n \geq 0. \quad (43)$$

Then for arbitrary  $f = (f_0, f_1, \dots, f_n, \dots)$ ,  $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$  according to definition (20) of the mapping  $\mathbb{E}xp_*$  the following equality holds

$$\mathfrak{d}_1(\mathbb{E}xp_* f) = \mathfrak{d}_1 f * \mathbb{E}xp_* f. \quad (44)$$

For  $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$  an analog of the annihilation operator is defined

$$(\mathfrak{a}f)_s(1, \dots, s) := \text{Tr}_{s+1} f_{s+1}(1, \dots, s, s+1), \quad (45)$$

and, therefore

$$(e^{\mathfrak{a}} f)_s(1, \dots, s) = \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{s+1, \dots, s+n} f_{s+n}(1, \dots, s, s+1, \dots, s+n), \quad s \geq 0.$$

Using previous definitions and (19) for sequences  $f^1 = (f_0^1, f_1^1, \dots, f_n^1, \dots)$ ,  $f_n^1 \in \mathfrak{L}^1(\mathcal{H}_n)$  and  $f^2 = (f_0^2, f_1^2, \dots, f_n^2, \dots)$ ,  $f_n^2 \in \mathfrak{L}^1(\mathcal{H}_n)$  we have [34]

$$(e^{\mathfrak{a}}(f^1 * f^2))_0 = (e^{\mathfrak{a}} f^1)_0 (e^{\mathfrak{a}} f^2)_0. \quad (46)$$

From equality (46) we deduce that expressions (39) and (40) can, respectively, be rewritten as

$$F_s(t, Y) = (e^{\mathfrak{a}} D(0))_0^{-1} (e^{\mathfrak{a}} \mathfrak{d}_{Y_1} D(t))_0$$

and

$$F_s(t, Y) = (e^{\mathfrak{a}} \mathfrak{d}_{Y_1} g(t))_0,$$

where  $Y = (1, \dots, s)$ .

Hence, in view of equalities (11), (21) to derive expressions (40) we have to prove the following lemma.

**Lemma 2.** For  $f = (f_0, f_1, \dots, f_n, \dots)$  and  $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$  the following identity holds

$$(e^{\mathfrak{a}} \mathbb{E} \exp_* f)_0^{-1} (e^{\mathfrak{a}} \mathfrak{D}_{Y_1} (\mathbb{E} \exp_* f))_0 = (e^{\mathfrak{a}} \mathfrak{D}_{Y_1} f)_0. \quad (47)$$

*Proof.* Indeed, using equalities (43), (44) and (46), we obtain

$$\begin{aligned} (e^{\mathfrak{a}} \mathbb{E} \exp_* f)_0^{-1} (e^{\mathfrak{a}} \mathfrak{D}_{Y_1} (\mathbb{E} \exp_* f))_0 &= (e^{\mathfrak{a}} \mathbb{E} \exp_* f)_0^{-1} (e^{\mathfrak{a}} (\mathbb{E} \exp_* f * \mathfrak{D}_{Y_1} f))_0 = \\ &= (e^{\mathfrak{a}} \mathbb{E} \exp_* f)_0^{-1} (e^{\mathfrak{a}} \mathbb{E} \exp_* f)_0 (e^{\mathfrak{a}} \mathfrak{D}_{Y_1} f)_0 = (e^{\mathfrak{a}} \mathfrak{D}_{Y_1} f)_0. \end{aligned}$$

□

## 5.2 On a solution of the BBGKY hierarchy

In this subsection we will turn to the solution of the initial-value problem of the BBGKY hierarchy. In the space  $\mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H}) = \bigoplus_{n=0}^{\infty} \alpha^n \mathfrak{L}^1(\mathcal{H}_n)$ , where  $\alpha > 1$  is a real number, we consider the following initial-value problem for the BBGKY hierarchy for quantum systems of particles obeying Maxwell-Boltzmann statistics

$$\begin{aligned} \frac{d}{dt} F_s(t) &= -\mathcal{N}_s F_s(t) + \\ &+ \sum_{n=1}^{\infty} \frac{1}{n!} \text{Tr}_{s+1, \dots, s+n} \sum_{\substack{Z \subset Y, \\ Z \neq \emptyset}} \left( -\mathcal{N}_{int}^{(|Z|+n)}(Z, s+1, \dots, s+n) \right) F_{s+n}(t), \end{aligned} \quad (48)$$

$$F_s(t) \big|_{t=0} = F_s(0), \quad s \geq 1, \quad (49)$$

where  $Y = (1, \dots, s)$  and the operator  $\mathcal{N}_{int}^{(n)}$  is defined on  $\mathfrak{L}_{\alpha,0}^1(\mathcal{F}_\mathcal{H}) \subset \mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})$  by formula (15). The equation from hierarchy (48) for  $s = 1$  has the following transparent form:

$$\frac{d}{dt} F_1(t) = -\mathcal{N}_1 F_1(t) + \sum_{n=1}^{\infty} \frac{1}{n!} \text{Tr}_{2, \dots, n+1} \left( -\mathcal{N}_{int}^{(n+1)}(1, 2, \dots, n+1) \right) F_{n+1}(t).$$

In the space  $\mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})$  there is an equivalent representation for the generator of the BBGKY hierarchy:

$$e^{\mathfrak{a}}(-\mathcal{N})e^{-\mathfrak{a}} = -\mathcal{N} + \sum_{n=1}^{\infty} \frac{1}{n!} [\dots [\mathcal{N}, \underbrace{\mathfrak{a}, \dots, \mathfrak{a}}_{n\text{-times}}]]$$

that follows from (39). For a two-body interaction potential one is reduced to the form [24]:  $-\mathcal{N} + [\mathcal{N}, \mathfrak{a}]$ .

We remark that in terms of the  $s$ -particle density matrix (marginal distribution)  $F_s(t, q_1, \dots, q_s; q'_1, \dots, q'_s)$  that are kernels of the  $s$ -particle density operators  $F_s(t)$ , for a two-body interaction potential (see (1) for  $k = 2$ ) the evolution operator (48) takes the canonical form of the quantum BBGKY hierarchy [10]

$$\begin{aligned} i\hbar \frac{\partial}{\partial t} F_s(t; q_1, \dots, q_s; q'_1, \dots, q'_s) &= \left( -\frac{\hbar^2}{2} \sum_{i=1}^s (\Delta_{q_i} - \Delta_{q'_i}) + \right. \\ &+ \sum_{i < j=1}^s (\Phi(q_i - q_j) - \Phi(q'_i - q'_j)) \Big) F_s(t; q_1, \dots, q_s; q'_1, \dots, q'_s) + \\ &+ \sum_{i=1}^s \int dq_{s+1} (\Phi(q_i - q_{s+1}) - \Phi(q'_i - q_{s+1})) F_{s+1}(t; q_1, \dots, q_s, q_{s+1}; q'_1, \dots, q'_s, q_{s+1}). \end{aligned}$$

For the solution of the BBGKY hierarchy the following theorem is true [25].

**Theorem 4.** *If  $F(0) \in \mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})$  and  $\alpha > e$ , then for  $t \in \mathbb{R}^1$  there exists a unique solution of initial-value problem (48)-(49) given by*

$$F_s(t, 1, \dots, s) = \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{s+1, \dots, s+n} \mathfrak{A}_{1+n}(t, Y_1, s+1, \dots, s+n) F_{s+n}(0, 1, \dots, s+n), \quad s \geq 1, \quad (50)$$

where for  $n \geq 0$

$$\mathfrak{A}_{1+n}(t, Y_1, s+1, \dots, s+n) = \sum_{P: \{Y_1, X \setminus Y\} = \bigcup_i X_i} (-1)^{|P|-1} (|P| - 1)! \prod_{X_i \subset P} \mathcal{G}_{|X_i|}(-t, X_i)$$

is the  $(1+n)$ th-order cumulant of operators (8),  $X \setminus Y = \{s+1, \dots, s+n\}$  and  $Y_1 = \{1 \cup \dots \cup s\}$ .

For initial data  $F(0) \in \mathfrak{L}_{\alpha,0}^1 \subset \mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})$  it is a strong solution and for arbitrary initial data from the space  $\mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})$  it is a weak solution.

The condition  $\alpha > e$  guarantees the convergence of series (50) and means that the average number of particles (10) is finite:  $\langle N \rangle < \alpha/e$ . This fact follows if to renormalize a sequence (50) in such a way:  $\tilde{F}_s(t) = \langle N \rangle^s F_s(t)$ .

For arbitrary  $F(0) \in \mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})$  the average number of particles (expectation value (10) expressed in terms of  $s$ -particle operators)

$$\langle N \rangle(t) = \text{Tr}_1 F_1(t, 1) \quad (51)$$

in state (50) is finite, in fact,

$$|\langle N \rangle(t)| \leq c_\alpha \|F(0)\|_{\mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})} < \infty,$$

where  $c_\alpha = e^2(1 - \frac{e}{\alpha})^{-1}$  is a constant. We emphasize the difference between finite and infinite systems with non-fixed number of particles. To describe an infinite particle system we have to construct a solution of initial-value problem (48)-(49) in more general spaces than  $\mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})$ , for example, in the space of sequences of bounded operators to which the equilibrium states belong [20, 34].

We remark that the formula for solution (50) can be directly derived from solution (28) of von Neumann hierarchy (12) [26]. In papers [2, 27, 32, 35] a solution of initial-value problem (48)-(49) is represented as the perturbation (iteration) series, which for a two-body interaction potential has the form

$$F_s(t) = \sum_{n=0}^{\infty} \int_0^t dt_1 \dots \int_0^{t_{n-1}} dt_n \text{Tr}_{s+1, \dots, s+n} \mathcal{G}_s(-t+t_1) \sum_{i_1=1}^s (-\mathcal{N}_{int}^{(2)}(i_1, s+1)) \mathcal{G}_{s+1}(-t_1+t_2) \times \dots \mathcal{G}_{s+n-1}(-t_{n-1}+t_n) \sum_{i_n=1}^{s+n-1} (-\mathcal{N}_{int}^{(2)}(i_n, s+n)) \mathcal{G}_{s+n}(-t_n) F_{s+n}(0). \quad (52)$$

In the space  $\mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})$  expansion (48) is equivalent to this iteration series. This follows from the validity of analogs of the Duhamel formula for cumulants of evolution operators of the von Neumann equations. For the second-order cumulant an analog of the Duhamel formula has the form (25) and in the general case the following formula takes place

$$\begin{aligned} \mathfrak{A}_{1+n}(t, Y_1, s+1, \dots, s+n) &= \\ &= \int_0^t dt_1 \dots \int_0^{t_{n-1}} dt_n \prod_{k_1 \in \mathcal{I}_1} \mathcal{G}_{|k_1|}(-t+t_1, k_1) \sum_{i_1 < j_1 \in \mathcal{I}_1} \sum_{l_1 \in i_1} \sum_{m_1 \in j_1} (-\mathcal{N}_{int}^{(2)}(l_1, m_1)) \times \\ &\quad \times \prod_{k_2 \in \mathcal{I}_2} \mathcal{G}_{|k_2|}(-t_1+t_2, k_2) \sum_{i_2 < j_2 \in \mathcal{I}_2} \sum_{l_2 \in i_2} \sum_{m_2 \in j_2} (-\mathcal{N}_{int}^{(2)}(l_2, m_2)) \times \dots \\ &\dots \times \prod_{k_n \in \mathcal{I}_n} \mathcal{G}_{|k_n|}(-t_{n-1}+t_n, k_n) \sum_{i_n < j_n \in \mathcal{I}_n} \sum_{l_n \in i_n} \sum_{m_n \in j_n} (-\mathcal{N}_{int}^{(2)}(l_n, m_n)) \mathcal{G}_{s+n}(-t_n, 1, \dots, s+n), \end{aligned}$$

where  $\mathcal{I}_1 \equiv \{Y_1, s+1, \dots, s+n\}$ ,  $\mathcal{I}_n \equiv \{i_{n-1} \cup j_{n-1}\} \cup \mathcal{I}_{n-1} \setminus \{i_{n-1}, i_{n-1}\}$ .

We remark that for classical systems of particles the first few terms of the cumulant expansion (50) were considered in [12].

In [25] we discuss other possible representations of a solution of the BBGKY hierarchy in the space  $\mathfrak{L}_\alpha^1(\mathcal{F}_\mathcal{H})$ .

### 5.3 Correlation operators of infinite-particle systems

Correlation operators (28) may be employed to directly calculate the macroscopic values of a system, in particular, fluctuations characterized by the average values of the square deviations of observables from its average values. For example, for an additive-type observable  $a = (a_0, a_1(1), \dots, \sum_{i=1}^n a_1(i), \dots)$  from the formula for expectation value (2) we derive the formula for fluctuations (the dispersion of an additive-type observable) [10]

$$\begin{aligned} \langle (a - \langle a \rangle(t))^2 \rangle(t) &= \\ &= \text{Tr}_1(a_1^2(1) - \langle a \rangle^2(t)) F_1(t, 1) + \text{Tr}_{1,2} a_1(1) a_1(2) (F_2(t, 1, 2) - F_1(t, 1) F_1(t, 2)). \end{aligned}$$

Therefore, the dispersion of the additive-type observable is defined not directly through the solutions of the BBGKY hierarchy but by the following correlation operators:  $F_2(t, 1, 2) - F_1(t, 1) F_1(t, 2) = G_2(t, 1, 2)$  or in the general case by the *s-particle correlation operators*

$$G_s(t, 1, \dots, s) := \sum_{\mathbf{P}: \{1, \dots, s\} = \bigcup_i X_i} (-1)^{|\mathbf{P}|-1} (|\mathbf{P}|-1)! \prod_{X_i \subset \mathbf{P}} F_{|X_i|}(t, X_i). \quad (53)$$

The *s*-particle correlation operators  $G_s(t)$ ,  $s \geq 1$  can be expressed in terms of correlation operators (28) by the formula

$$G_s(t, 1, \dots, s) = \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{s+1, \dots, s+n} g_{s+n}(t, 1, \dots, s+n), \quad s \geq 1, \quad (54)$$

where  $g_{s+n}(t, 1, \dots, s+n)$  is a solution of the von Neumann hierarchy (12).

To derive expression (54) we state the following lemma.

**Lemma 3.** *Let  $f = (f_0, f_1, \dots, f_n)$  and  $f_n \in \mathfrak{L}^1(\mathcal{H}_n)$ , then the equality holds*

$$(e^a \mathbb{E} \exp_* f)_0^{-1} e^a \mathbb{E} \exp_* f = \mathbb{E} \exp_* e^a f.$$

*Proof.* Indeed, using equality (46) and the equality

$$\mathfrak{d}_1 \dots \mathfrak{d}_s \mathbb{E} \exp_* f = \mathbb{E} \exp_* f * \sum_{P: Y = \bigcup_i X_i} \mathfrak{d}_1 \dots \mathfrak{d}_{|X_1|} f * \dots * \mathfrak{d}_{|X_{|P|-1}|+1} \dots \mathfrak{d}_{|X_{|P|}|} f,$$

that follows from (42), (44), one obtains (here  $Y = (1, \dots, s)$ )

$$\begin{aligned} (e^a \mathbb{E} \exp_* f)_0^{-1} (e^a \mathbb{E} \exp_* f)_{|Y|}(Y) &= (e^a \mathbb{E} \exp_* f)_0^{-1} (e^a \mathfrak{d}_1 \dots \mathfrak{d}_s (\mathbb{E} \exp_* f))_0 = \\ &= (e^a \mathbb{E} \exp_* f)_0^{-1} \left( e^a (\mathbb{E} \exp_* f * \sum_{P: Y = \bigcup_i X_i} \mathfrak{d}_1 \dots \mathfrak{d}_{|X_1|} f * \dots * \mathfrak{d}_{|X_{|P|-1}|+1} \dots \mathfrak{d}_{|X_{|P|}|} f) \right)_0 = \\ &= (e^a \mathbb{E} \exp_* f)_0^{-1} (e^a \mathbb{E} \exp_* f)_0 \left( e^a \sum_{P: Y = \bigcup_i X_i} \mathfrak{d}_1 \dots \mathfrak{d}_{|X_1|} f * \dots * \mathfrak{d}_{|X_{|P|-1}|+1} \dots \mathfrak{d}_{|X_{|P|}|} f \right)_0 = \\ &= \sum_{P: Y = \bigcup_i X_i} \prod_i (e^a \mathfrak{d}_1 \dots \mathfrak{d}_{|X_i|} f)_0 = (\mathbb{E} \exp_* e^a f)_{|Y|}(Y). \end{aligned}$$

□

We now derive representation (54) for  $s$ -particle correlation operators. Using equality (11) in terms of the mapping  $\mathbb{E} \exp_*$  (20), representation (39) for  $s$ -particle statistical operators can be rewritten in the form

$$F(t) = (e^a \mathbb{E} \exp_* g(0))_0^{-1} e^a \mathbb{E} \exp_* g(t).$$

In terms of the mapping  $\mathbb{E} \exp_*$  formula (53) has the form

$$F(t) = \mathbb{E} \exp_* G(t).$$

Further, according to previous formula and Lemma 3 we have

$$\mathbb{E} \exp_* G(t) = (e^a \mathbb{E} \exp_* g)_0^{-1} e^a \mathbb{E} \exp_* g(t) = \mathbb{E} \exp_* e^a g(t),$$

and, therefore, we finally derive

$$G(t) = e^a g(t) \tag{55}$$

or in component-wise form (54).

For chaos initial data (30) obeying Maxwell-Boltzmann statistics according to (55) we have  $G_1(0) = g_1(0)$ . Using solution (31) of the von Neumann hierarchy (12) the expansion for a solution of the initial-value problem for  $s$ -particle correlation operators can be represented as follows

$$G_s(t, 1, \dots, s) = \sum_{n=0}^{\infty} \frac{1}{n!} \text{Tr}_{s+1, \dots, s+n} \mathfrak{A}_{s+n}(t, 1, \dots, s+n) \prod_{i=1}^{s+n} G_1(0, i), \quad s \geq 1.$$

It should be noted that sequence (55) is a solution of the nonlinear BBGKY hierarchy for  $s$ -particle correlation operators [29] which describes the dynamics of correlations of infinite-particle systems.

## Acknowledgement

This work was partially supported by the WTZ grant No M/124 (UA 04/2007) and by the Special programm of the PAD of NAS of Ukraine.

## References

- [1] Adami R, Bardos C, Golse F, Teta A 2004 Towards a rigorous derivation of the cubic nonlinear Schrödinger equation in dimension one *Asymptot. Anal.* **40** (2) 93-108
- [2] Arnold A 2008 Mathematical properties of quantum evolution equations *to appear in Lecture Notes in Mathematics*, (Berlin: Springer)
- [3] Banasiak J, Arlotti L 2006 *Perturbations of Positive Semigroups with Applications* (Berlin: Springer) p 438
- [4] Bardos C, Ducomet B, Golse F, Gottlieb A, Mauser N 2007 The TDHF approximation for Hamiltonians with m-particle interaction potentials *Commun. in Math. Sci.* **5** 1 - 9
- [5] Bardos C, Golse F, Gottlieb A and Mauser N 2003 Mean field dynamics of fermions and the time-dependent Hartree-Fock equation *J. Math. Pures et Appl.* **82** 665–683
- [6] Benedetto D, Castella F, Esposito R and Pulvirenti M 2007 A short review on the derivation of the nonlinear quantum Boltzmann equations *Commun. Math. Sci.* **5** 55–71.
- [7] Benedetto D, Castella F, Esposito R and Pulvirenti M 2004 Some consideration on derivation nonlinear quantum Boltzmann equation *J. Stat. Phys.* **116**(1/4) 381-410
- [8] Benedetto D, Castella F, Esposito R, Pulvirenti M 2006 Some considerations on the derivation of the nonlinear quantum Boltzmann equation II: the low density regime *J. Stat. Phys.* **124** (2-4) 951-996
- [9] Berezin F A, Shoubin M A 1991 *Schrödinger Equation* (Amsterdam: Kluwer) p 576
- [10] Bogolyubov N N 1949 *Lectures on Quantum Statistics*. (Kyiv: Rad. shkola) p 227 (in Ukrainian)
- [11] Cercignani C, Gerasimenko V I, Petrina D Ya 1997 *Many-Particle Dynamics and Kinetic Equations* (Dordrecht: Kluwer Acad. Publ.) p 252
- [12] Cohen E G D 1968 The kinetic theory of dense gases 228-275 in *Fundamental Problems in Statistical Mechanics II* (ed. E. G. D. Cohen. – Amsterdam: North-Holland)
- [13] Dautray R and Lions J L 1992 *Mathematical Analysis and Numerical Methods for Science and Technology* vol 5 ( Berlin: Springer-Verlag) p 562
- [14] Elgart A, Schlein B Mean field dynamics of boson stars 2007 *Comm. Pure Applied Math.* **60** (4) 500-545



- 
- [15] Erdős L, Salmhofer M and Yau H-T 2004 On quantum Boltzmann equation *J. Stat. Phys.* **116** (116) 367-380
  - [16] Erdős L, Schlein B, Yau H-T 2007 Rigorous derivation of the Gross-Pitaevskii equation *Phys. Rev. Lett.* **98**. (4) 040404
  - [17] Erdős L, Schlein B, Yau H-T 2006 Derivation of the Gross-Pitaevskii hierarchy for the dynamics of a Bose-Einstein condensate *Comm. Pure Applied Math.* **59** (12) 1659-1741
  - [18] Erdős L, Schlein B, Yau H-T 2007 Derivation of the cubic nonlinear Schrödinger equation from quantum dynamics of many-body systems *Invent Math.* **167** (3) 515-614
  - [19] Fröhlich J, Lenzmann E 2005 Nonlinear Equations describing the Mean-Field Limit of Bose Gases *Workshop: Math. Methods in Quantum Mechanics, Bressanone* p 25
  - [20] Genibre J 1971 Some applications of functional integrations in statistical mechanics 329-427 in *Statistical Mechanics and Quantum Field Theory* (eds. S. de Witt and R. Stord - N.Y.: Gordon and Breach)
  - [21] Gerasimenko V I, Petrina D Ya 1997 On generalized kinetic equation *Reports of NAS of Ukraine* **7** 7-12 (in Ukrainian)
  - [22] Gerasimenko V I and Ryabukha T V 2002 Cumulant representation of solutions of the BBGKY hierarchy of equations *Ukrainian Math. J.* **54**(10) 1583-1601
  - [23] Gerasimenko V I, Shtyk V O 2008 Bogolyubov decay of correlations principle for infinite system of hard spheres *to appear in Reports of NAS of Ukraine*, **3** (in Ukrainian)
  - [24] Gerasimenko V I and Shtyk V O 2007 The Cauchy problem for the nonlinear von Neumann hierarchy *Proceedings of Institute of Mathematics of NASU* **4** (3) 27-51 (in Ukrainian)
  - [25] Gerasimenko V I and Shtyk V O 2006 Initial-value problem for the Bogolyubov hierarchy for quantum systems of particles *Ukrainian Math. J.* **58** (9) 1175-1191
  - [26] Gerasimenko V I, Shtyk V O 2006 Existence criterion of cumulant representation for solution of initial value problem of quantum BBGKY hierarchy *Reports of NAS of Ukraine* **8** 42-49 (in Ukrainian)
  - [27] Golse F 2003 The mean-field limit for the dynamics of large particle systems *Journées equations aux dérivées partielles* **9** p 47
  - [28] Gottlieb A D and Mauser N J 2005 New measure of electron correlation *Phys. Rev. Lett.* **95** (12) 213-217.
  - [29] Green M S 1956 Boltzmann equation from the statistical mechanical point of view *J. Chem. Phys.* **25** (5) 836-855
  - [30] Kato T 1995 *Perturbation Theory for Linear Operators* (Berlin: Springer-Verlag) p 619

- 
- [31] Markowich P A, Ringhofer C and Schmeiser C 1990 *Semiconductor Equations* (Berlin: Springer) p 248
  - [32] Petrina D Ya 1972 On solutions of Bogolyubov kinetic equations. *Quantum statistics Theor. and Math. Phys.* **13**(3) 391-405
  - [33] Petrina D Ya 1995 *Mathematical Foundations of Quantum Statistical Mechanics. Continuous Systems* (Amsterdam: Kluwer) p 624
  - [34] Ruelle D 1999 *Statistical Mechanics. Rigorous Results* (Singapur: World Sci. Publ. Co.) p 314
  - [35] Schlein B 2006 Derivation of the Gross-Pitaevskii hierarchy *Mathematical Physics of Quantum Mechanics, Lecture Notes in Physics 690* (Springer(Proceedings of QMath 9))
  - [36] Spohn H 2007 Kinetic equations for quantum many-particle systems *arXiv:0706.0807v1*
  - [37] Shtyk V O 2007 On the solutions of the nonlinear Liouville hierarchy *J. Phys. A: Math. Theor.* **40** 9733-9742